

Formyl chloride
2565-30-2 | DTXSID30180344

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 50.3 °C

Global applicability domain: Inside

Local applicability domain index: 5.88e-01

Confidence level: 7.98e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Acetaldehyde</div> <div>Measured: 20.1</div> <div>Predicted: 23.9</div>	<div>Image not found</div> <div>Acetyl chloride</div> <div>Measured: 50.7</div> <div>Predicted: 59.4</div>	<div>Image not found</div> <div>Propanal</div> <div>Measured: 48.0</div> <div>Predicted: 47.1</div>
<div>Image not found</div> <div>Acetone</div> <div>Measured: 55.8</div> <div>Predicted: 48.2</div>	<div>Image not found</div> <div>(2H6)Acetone</div> <div>Measured: 55.8</div> <div>Predicted: 50.0</div>	<div>Image not found</div> <div>Chloroacetaldehyde</div> <div>Measured: 85.5</div> <div>Predicted: 86.0</div>